The Quantum Dynamics of Polaron Formation

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When degrees of freedom interact, they can form composite objects called quasiparticles. An example is the coupling of an electron with phonons, forming a polaron quasiparticle. A polaron is an electron traveling with a cloud of lattice distortions, which can have a mass slightly greater or orders of magnitude greater than a bare electron, depending on the strength of the coupling. By efficiently organizing the many-body Hilbert space, we have calculated the energy, mass, and correlation functions of the polaron many orders of magnitude more accurately than was previously possible. Other types of quasiparticles arise in different contexts, including interactions of electrons with magnetism, with other electrons, etc.

We investigate how a bare electron, injected by fast optical processes or by a tunneling event, dynamically becomes a polaron quasiparticle (plus unbound phonons). The phonons and electrons are treated quantum mechanically. (Treating the phonons classically, a common approximation, fails to capture some of the physics.) The method used is to numerically integrate the time-dependent Schrödinger equation in a many-body Hilbert space of over a million basis states. Various time and position-dependent correlation functions have been calculated and displayed as a movie, frames from which are shown in the figure. Depending on the parameters (the electron-phonon coupling, the optical phonon frequency, and the electron hopping), the polaron can form in a time as short as a phonon period, or arbitrarily longer. The spectral function and other time-dependent correlation functions have also been calculated, and compared to fast optical and two-photon photoemission experiments [1].

The figure shows four snapshots from a movie of a polaron quasiparticle forming from a bare electron. In panel (a), a bare electron is injected moving to the right, with the electron density shown in black. The electron velocity (green) is positive. The phonon displacement $<X_j>$ (red) is initially zero. (For clarity, the red and green curves have been shifted upwards by 0.1.) At time 0.5, panel (b), the phonons are displaced where the initial electron was injected. At time 1.0, panel (c), the electron density (black) has developed two peaks. The peak on the right is a bare electron, moving quickly. The peak on the left is a slower and more massive electron dressed with phonon excitations, the polaron quasiparticle. The phonon displacement (red) is oscillating and is now negative where the electron was initially injected, but it is positive to the right where the electron arrived later. Also shown are the electron density that would have been present if there were no coupling to the phonons (dashed black line), and the phonon number density (blue). The magenta curve plots the phonon number density on the electron site j, $<c_j^\dagger a_j^\dagger a_j>$. The green curve shows that some electron density has been backscattered, and is moving to the left, at the left side of the frame. Panel (d), at time 1.5, shows the bare electron peak getting smaller with time (black arrow), while the polaron peak grows as time goes on (red arrow). Most of the phonons were radiated near where the electron was initially injected (blue). (Note that the phonons are dispersionless optical phonons in this simulation, so they do not move unless the electron is nearby.) The displacement of the oscillating phonons has reversed yet again (red curve). The simulation is for a 30-site system with periodic boundary conditions.

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[1] Li-Chung Ku and S.A. Trugman, "Quantum Dynamics of Polaron Formation," submitted to *Phys. Rev. Lett.*, 2005.

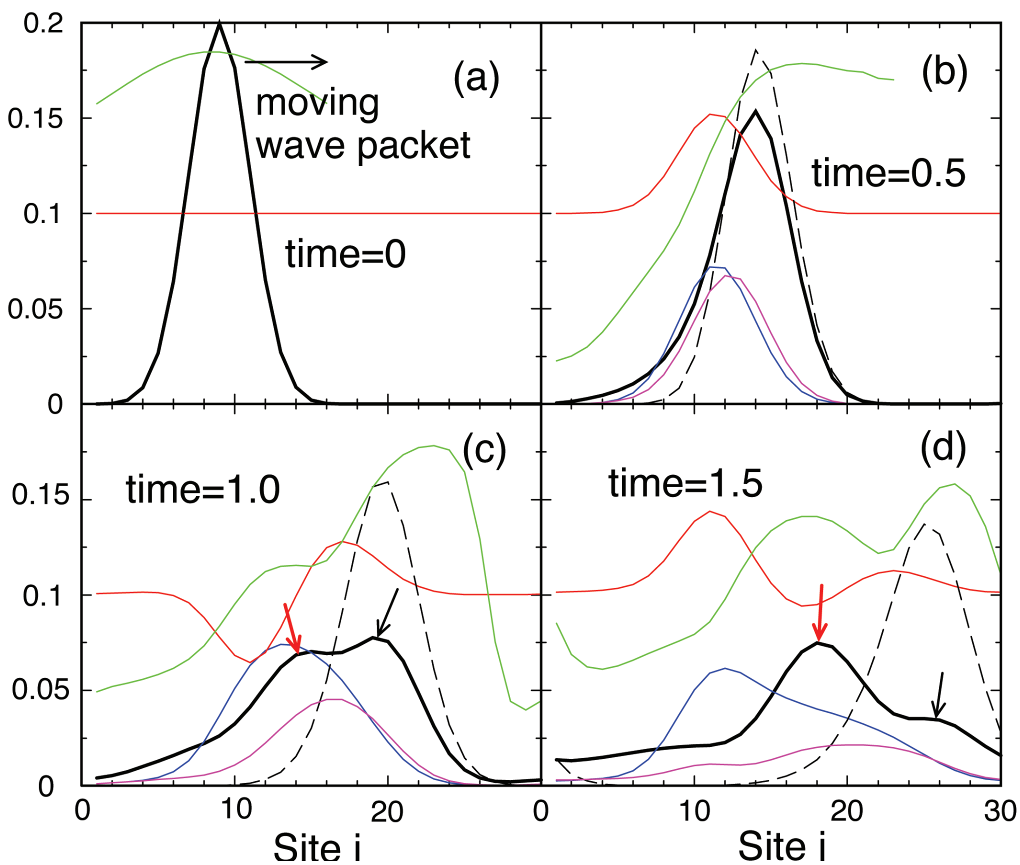

Fig. 1.
Four snapshots from a movie of a polaron quasiparticle forming from a bare electron. The electron and phonons are all treated quantum mechanically. Time is measured in units of the phonon vibrational period.